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FILE 'HOME' ENTERED AT 19:29:07 ON 14 NOV 2004

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0.21

0.21

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STRUCTURE FILE UPDATES: 12 NOV 2004 HIGHEST RN 780001-49-2  
DICTIONARY FILE UPDATES: 12 NOV 2004 HIGHEST RN 780001-49-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

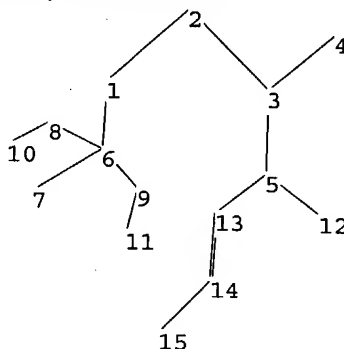
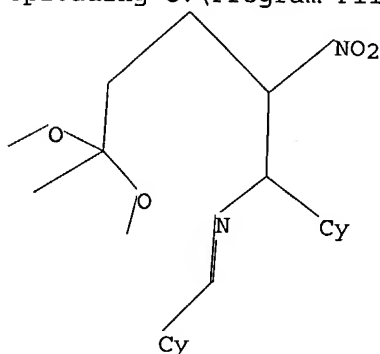
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=>

Uploading C:\Program Files\Stnexp\Queries\10705466.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

chain bonds :

1-2 1-6 2-3 3-4 3-5 5-12 5-13 6-7 6-8 6-9 8-10 9-11 13-14 14-15

exact/norm bonds :

5-12 5-13 6-8 6-9 8-10 9-11 13-14 14-15

exact bonds :

1-2 1-6 2-3 3-4 3-5 6-7

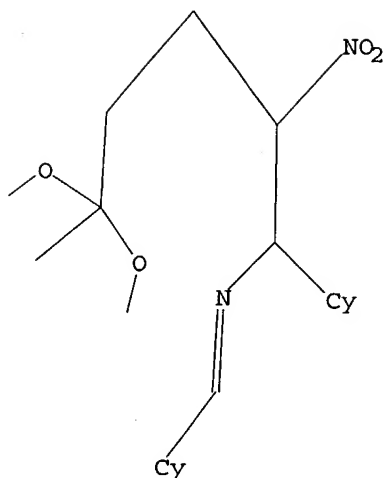
Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS 15:Atom

L1 STRUCTURE UPLOADED

=> d query

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 19:29:31 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 0 TO 0  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 19:29:34 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01

L3 2 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
155.42	155.63

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FILE 'CAPLUS' ENTERED AT 19:29:37 ON 14 NOV 2004  
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FILE COVERS 1907 - 14 Nov 2004 VOL 141 ISS 21  
FILE LAST UPDATED: 12 Nov 2004 (20041112/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 2 L3

=> d l4 1-2 abs ibib hitstr

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
 AB This document discloses a process for preparing a pure cis isomer from a mixture of cis-trans isomers of formula  $RC(OMe)2CH2CH2CH(NO2)CH(Ar)N:CHAr$  (I) [Ar = (un)substituted Ph, etc.; R = alkyl] comprising the steps of: (a) dispersing a mixture of cis- and trans-I in an inert solvent wherein said cis isomer is less soluble than said trans isomer; (b) heating said dispersion to completely dissolve said trans isomer; (c) maintaining said heating step to allow interconversion of said cis and trans isomer; (d) cooling said mixture thereby crystallizing the cis isomer; (e) separating said crystalline cis isomer from said solvent. Cis isomers of formula I are useful intermediates in the synthesis of cis isomers of benzamide piperidine compds. which exhibit activity as NK-1 receptor antagonists.

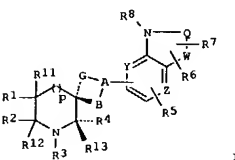
ACCESSION NUMBER: 2004:428898 CAPLUS  
 DOCUMENT NUMBER: 141:6912  
 TITLE: Process for converting a cis-trans mixture of substituted benzylidene amines into the pure cis isomer  
 INVENTOR(S): Humphrey, John Michael; Tom, Norma Jacqueline  
 PATENT ASSIGNEE(S): Pfizer Products Inc., USA  
 SOURCE: PCT Int. Appl., 21 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004043908	A1	20040527	WO 2003-1B4953	20031103
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: BW, CH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.: US 2002-425946P P 20021112				

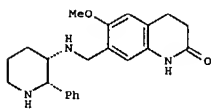
OTHER SOURCE(S): CASREACT 141:6912; MARPAT 141:6912  
 IT 695165-42-5P  
 RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)  
 (process for converting a cis-trans mixture of substituted benzylidene amines into the pure cis isomer)  
 RN 695165-42-5 CAPLUS  
 CN Benzenemethanamine,  $\alpha$ -(4,4-dimethoxy-1-nitrohexyl)-N-(phenylmethylene)-, [N(Z)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
 GI



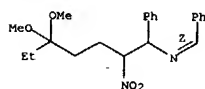
I



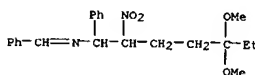
II

AB Title compds. I [Q = C:NH, C:CH2, C:S, C:O, SO, SO2; A = CH, CH2, C(alkyl), CH(alkyl), C(CF3), or CH(CF3) with the proviso that when B is present, A = CH, C(alkyl), or C(CF3); B = absent, CH2, or ethylene; Y, Z = N, CH, provided that both are not N; G = NH(CH2)q, S(CH2)q, O(CH2)q; q = 0-1 with the proviso that when q = 0, G = NH2, SH, OH; W = 1-3 carbon linking group, including spiro assemblies; p = 0-2; R3 = H, acyl, carboxy, Ph, heterocyclyl, alkyl, etc.; R1, R2, R11-13 = H, alkyl, etc., or R12-13 together with the carbon atoms to which they are attached form a 5- or 6-membered heterocyclic ring, etc.; R4 = Ph, pyridyl, thienyl, etc.; R5-8 = H, alkyl, S(O)1-2-alkyl, alkoxy, halo, Ph, etc.] were prepared. Approx. 100 synthetic examples and over 100 precursor preps. were provided. For instance, 4-aminophenol was acylated with 3-chloropropionyl chloride (CH2Cl2, H2O, NaHCO3, room temperature, 4 h) and the product treated with AlCl3 at 210°C for 10 min effecting cyclization to the hydroxy quinoline intermediate. The intermediate was O-methylated (acetone, Me2SO4, K2CO3, room temperature, 16 h) and formulated in the 7 position (CH2Cl2, AlCl3, Cl2CHOMe) to give 7-formyl-6-methoxy-1H-1,2,3,4-tetrahydroquinolin-2-one. Reductive alkylation of the quinoline with (2S,3S)-3-amino-2-phenylpiperidine (a. PhMe, 3A mol. sieves; B. dichloroethane, NaBH(OAc)3, room temperature, 16 h) yielded II. Compds. I are NK-1 receptor antagonists, i.e., substance P receptor antagonists. At least one

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT 368835-48-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (process for converting a cis-trans mixture of substituted benzylidene amines into the pure cis isomer)  
 RN 368835-48-7 CAPLUS  
 CN Benzenemethanamine,  $\alpha$ -(4,4-dimethoxy-1-nitrohexyl)-N-(phenylmethylene)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
 stereoisomer of the example compds. had a binding affinity, as measured by

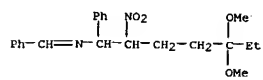
Ki, of at least 600 nM. I are used in the treatment and prevention of a wide variety of central nervous system disorders, inflammatory disorders, cardiovascular disorders, ophthalmic disorders, etc.

ACCESSION NUMBER: 2001:762988 CAPLUS  
 DOCUMENT NUMBER: 135:331346  
 TITLE: Synthesis of benzoamide piperidine containing compounds as substance P antagonists  
 INVENTOR(S): Arnold, Eric Platt; Chappie, Thomas Allen; Huang, Jianhua; Humphrey, John Michael; Nagel, Arthur Adam; O'Neill, Brian Thomas; Sobolov-Jaynes, Susan Beth; Vincent, Lawrence Albert  
 PATENT ASSIGNEE(S): Pfizer Products Inc., USA  
 SOURCE: PCT Int. Appl., 209 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077100	A2	20011018	WO 2001-1B629	20010406
WO 2001077100	A3	20020307		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG US 2003087925 A1 20030508 US 2001-811218 20010316 EP 1272484 A2 20030308 EP 2001-919702 20010406 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR BR 2001009936 A 20030506 BR 2001-9936 20010406 JP 200401072 T2 20040115 JP 2001-575573 20010406 EE 200200588 A 20040415 EE 2002-588 20010406 NZ 521346 A 20040730 NZ 2001-521346 20010406 BG 107135 A 20030630 BG 2002-107135 20020923 ZA 2002008072 A 20031008 ZA 2002-8072 20021008 NO 2002004874 A 20021118 NO 2002-4874 20021009 PRIORITY APPLN. INFO.: US 2000-195922P P 20000410 US 2000-212922P P 20000620 WO 2001-1B629 W 20010406				

OTHER SOURCE(S): MARPAT 135:331346  
 IT 368835-48-7P, Benzylidene-(5,5-dimethoxy-2-nitro-1-phenylheptyl)amine  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; synthesis of benzoamide piperidine containing compds. as substance P antagonists)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
 RN 368835-48-7 CAPLUS  
 CN Benzenemethanamine,  $\alpha$ -(4,4-dimethoxy-1-nitrohexyl)-N-(phenylmethylene)- (9CI) (CA INDEX NAME)



=> logoff y  
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
11.28	166.91

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
-1.40	-1.40

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